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Point and space groups and elastic behaviours of one-dimensional quasicrystals

Renhui Wang, Wenge Yang, Chengzheng Hu and Di-hua Ding
Department of Physics, Wuhan University, 430072 Wuhan, People's Republic of China

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Abstract. A one-dimensional (1D) quasicrystal (QC) is defined as a three-dimensional body which is periodic in the x–y plane and quasiperiodic in the third dimension. Knowing that the possible symmetry operations for a 1D QC are $1, 2, 3, 4, 6, m, \bar{1}$ (inversion), 2_h (horizontal twofold rotation) and m_h (horizontal mirror reflection), 31 possible point groups of 1D QCs have been deduced. These 31 point groups are divided into ten Laue classes and six systems. Considering screw (only 2_{1h}) and glide (only a, b and n_h) operations, 80 possible space groups of 1D QCs have also been obtained. According to our generalized elasticity theory of QCs, the elastic behaviours, including independent elastic constants and invariants, for each Laue class of 1D QCs have been discussed.

1. Introduction

Since the discovery of three-dimensional (3D) icosahedral quasicrystal (QCs) in Al–Mn alloys (Shechtman *et al* 1984), 3D cubic QCs (Feng *et al* 1989, Wang *et al* 1994), two-dimensional (2D) QCs (Bendersky 1985, Ishimasa *et al* 1985, Wang *et al* 1987), and one-dimensional (1D) QCs have been discovered in succession. A 1D QC is defined as a 3D body which is periodic in the x–y plane and quasiperiodic in the third direction. Merlin *et al* (1985), Hu *et al* (1986), Feng *et al* (1987), Terauchi *et al* (1988) and Chen *et al* (1987, 1989) prepared a Fibonacci sequence with alternating layers of GaAs and AlAs or $Al_{0.5}Ga_{0.5}As$, where the GaAs and AlAs were grown by molecular-beam epitaxy. He *et al* (1988) found a 1D QC derived from the 2D decagonal QC in rapidly solidified Al–Ni–Si, Al–Cu–Mn, and Al–Cu–Co alloys. Tsai *et al* (1992) and Yang *et al* (1996) reported the discovery of some stable 1D QCs in the Al–Cu–Fe–Mn system. There have also been some theoretical studies about 1D QCs; Miyazaki and Inoue (1990) calculated the optical reflectivity of the semiconductor Fibonacci superlattice. Lele and Mandal (1990) proposed a method of generating a 1D QC by distorting the six-dimensional supercubic lattice and the icosahedral basis vectors along the threefold axis. The point group of such a 1D QC is $\bar{3}$. Zhang and Kuo (1990) described various 1D QCs by adding linear phason strain to the decagonal QCs. All the 1D QCs related to decagonal QCs (He *et al* 1988, Zhang and Kuo 1990, Tsai *et al* 1992) belong to the orthorhombic system. One may ask how many point groups, space groups and systems can exist for 1D QCs. In sections 2 and 3, we derive all the possible point and space groups of 1D QCs.

The field of linear elasticity theory of QCs has been investigated for years. Levine *et al* (1985) and Socolar (1989) derived expressions for quadratic invariants and elastic energies of icosahedral and planar pentagonal, octagonal and dodecagonal QCs. Ding *et al* (1993)

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proposed a generalized elasticity theory and obtained Hooke's law and the equilibrium equations for QCs. Yang *et al* (1993) discussed the linear elasticity equations and elastic energy for the cubic QS. Yang *et al* (1995a, b) and Hu *et al* (1996) discussed the linear elastic behaviour of 2D QCs. Nevertheless, there has been no systematic report in this field for 1D QCs. In section 4, we shall discuss the elastic behaviour, including independent elastic constants and invariants, for each point group of the 1D QCs. Some discussion is given in section 5.

2. Possible point groups for one-dimensional quasicrystals

The possible symmetry elements for 1D QCs are the n and $\bar{n}$ axes ($n = 1, 2, 3, 4$ and 6) along the z direction which is perpendicular to the x–y periodic plane, and also the twofold axes 2_h (horizontal twofold rotation) and $\bar{2}_h = m$ (vertical mirror reflection) in the periodic plane. Other axes ($n = 5, 7, 8, \ldots$) are incompatible with the periodicity in the x–y plane. Moreover, any axis, except $1, \bar{1}$ and the horizontal twofold axes 2_h and $\bar{2}_h = m$, must be perpendicular to the periodic x–y plane. Otherwise the periodicity in the x–y plane would be transformed to the third direction outside the x–y plane and the studied body would become a 3D crystal. The point symmetry operations for 1D QCs may be divided into two types for which the first-type operations are proper rotations n ($n = 1, 2, 3, 4$ and 6) about the vertical axis and reflections m across vertical mirror planes, and each second-type operation is a compound operation which is a product of inversion $\bar{1}$ and one of the first-type operations. For example, the following operations belong to the second type: $m_h = \bar{1} \cdot 2 = \bar{2}$, $\bar{n} = \bar{1} \cdot n$ ($n = 3, 4, 6$), $1_h = \bar{1} \cdot m$.

It is well known (Wang and Kuo 1990) that point groups consisting of only the first-type operations 1, 2, 3, 4, 6 and m are the following ten 2D crystallographic point groups:

$$1, 2, 3, 4, 6, m, 2mm, 3m, 4mm, 6mm \tag{1}$$

which are listed in the first column of table 1. In the present paper we use the conventional Hermann–Mauguin symbols (Hahn 1983) to describe the point and space groups.

Table 1. Derivation of 31 point groups for 1D QCs (S represents subgroup of index 2 of H).

H	$\{1, \bar{1}\} \otimes H$	S	$H' = S + \bar{1}\{H/S\}$
1	$\bar{1}$	—	—
2	$2/m_h$	1	m_h
3	$\bar{3}$	—	—
4	$4/m_h$	2	$\bar{4}$
6	$6/m_h$	3	$\bar{6}$
m	$2_h/m$	1	2_h
$2mm$	mmm_h	2	$2_h 2_h 2$
		m	$2_h mm_h$
$3m$	$\bar{3}m$	3	32_h
$4mm$	$4/m_h mm$	4	$42_h 2_h$
		$2mm$	$\bar{4}2_h m$
$6mm$	$6/m_h mm$	6	$62_h 2_h$
		$3m$	$\bar{6}m2_h$

Since the product of any two second-type operations is a first-type operation, we conclude from group theory (Wang and Kuo 1990) that any group H' containing second-type operations has a subgroup S of index 2 which consists of all the first-type operations

in the group H':

$$H' = S + (H'/S) \tag{2}$$

where

$$H' = \{1, h_2, \ldots, h_s, h'_{s+1}, \ldots, h'_{2s}\}$$
$$S = \{1, h_2, \ldots, h_s\}$$

and

$$H'/S = \{h'_{s+1}, h'_{s+2}, \ldots, h'_{2s}\} = h'_{s+j}S \tag{3}$$

with $h'_{s+j} = \bar{1} \cdot h_{s+j}$ $(j = 1, 2, \ldots, s) \in H'/S$ being second-type operations and h_{s+j} their corresponding first-type operations.

When some h'_{s+j} in equation (3) itself is an inversion operation $\bar{1}$, then we can rewrite (2) as a direct product:

$$H' = S \times \{1, \bar{1}\} \tag{4}$$

where S is one of the 2D crystallographic point groups listed in (1). Hence we can derive ten point groups for 1D QCs as follows:

$$\bar{1}, 2/m_h, \bar{3}, 4/m_h, 6/m_h, 2_h/m, mmm_h \left(= \frac{2_h}{m}\frac{2_h}{m}\frac{2}{m_h}\right), \bar{3}m \left(= \bar{3}\frac{2_h}{m}\right),$$
$$4/m_hmm \left(= \frac{4}{m_h}\frac{2_h}{m}\frac{2_h}{m}\right), 6/m_hmm \left(= \frac{6}{m_h}\frac{2_h}{m}\frac{2_h}{m}\right) \tag{5}$$

which are listed in the second column of table 1.

When the coset H'/S in (3) does not contain the inversion operation $\bar{1}$, then we can conclude from group theory (Wang and Kuo 1990) that the group

$$H = \{1, h_2, \ldots, h_s, h_{s+1}, \ldots, h_{2s}\} \tag{6}$$

is isomorphic to H'. Hence we can derive other point groups for 1D QCs by finding subgroups S of index 2 from the ten point groups H as listed in the third column of table 1, and then changing all the operations $h_{s+j} \in H/S$ into corresponding second-type operations $h'_{s+j} = \bar{1} \cdot h_{s+j}$. In this way we obtain the other 11 point groups:

$$m_h, \bar{4}, \bar{6}, 2_h, 2_h2_h2, 2_hmm_h, 32_h, 42_h2_h, \bar{4}2_hm, 62_h2_h, \bar{6}m2_h \tag{7}$$

which are listed in the fourth column of table 1.

These 31 point groups for 1D QCs may also be derived by the following considerations. The possible operations $n, \bar{n}$ ($n = 1, 2, 3, 4$ and 6), 2_h and $\bar{2}_{h\cdot} = m$ for 1D QCs all belong to crystallographic point operations; hence any point group of 1D QCs must be one of the 32 crystallographic point groups. By excluding five cubic point groups $23, m\bar{3}, 432, \bar{4}3m$ and $m\bar{3}m$ which contain oblique axes and considering 2 and 2_h, m and $m_{h\cdot}$, $2/m_h$ and $2_h/m$, $2mm$ and 2_hmm_h as different point groups, we again obtain 31 point groups for 1D QCs.

These 31 point groups may be divided into six systems and ten Laue classes as shown in the first three columns of table 2. According to Yang *et al* (1995a), the elastic behaviours are the same for point groups belonging to the same Laue class.

3. Possible space groups for one-dimensional quasicrystals

Since a 1D QC allows translations only along the x–y periodic plane, the allowable centring types are primitive (P) and C-face-centred (C) cells. Moreover, besides the point symmetry elements $n, \bar{n}, 2_h$ and m mentioned in section 2, other allowable elements are horizontal twofold screw axes $2_1[100]$ and $2_1[010]$, vertical glide planes $a[010]$ and $b[100]$, and also horizontal glide planes $a[001]$, $b[001]$ and $n[001]$. Therefore, space groups for 1D QCs are selected from 230 3D crystallographic space groups (Hahn 1983) according to the following procedures:

(1) Exclude all the cubic space groups because they contain oblique axes.

(2) For each monoclinic and orthorhombic space group, consider various settings (Hahn 1983) of the same unit cell. For example, for the space group $Pmna$ No (53), consider also its other settings: $Pnmb$, $Pbmn$, $Pcnm$, $Pncm$ and $Pman$, which are not equivalent for 1D QCs.

(3) Exclude all the space groups of A-face-; B-face-; body- and all-face-centred and rhombohedral (R) cells, and all the space groups containing intrinsic translations along the z direction, e.g. $n[010](t = [1/2, 0, 1/2])$ and $n[100](t = [0, 1/2, 1/2])$. Hence, the above space groups $Pmna$, $Pnmb$, $Pcnm$ and $Pncm$ are excluded and only $Pbmn$ and $Pman$ remain as space groups of 1D QCs.

In this way we have derived 80 space groups for 1D QCs as listed in the fifth column of table 2. The sixth column lists the sequence numbers of these space groups in the *International Tables for Crystallography* (Hahn 1983).

It should be noted that these 80 space groups for 1D QCs are exactly the layer groups G_2^3 as discussed by Vainshtein (1981) and Wang and Kuo (1990).

4. Linear elasticity behaviour of one-dimensional quasicrystals

In the case of crystals, all order invariants of all crystal classes can be easily obtained according to group representation theory and have been tabulated by Teodosiu (1982). In section 2, we have derived all the possible 31 point groups of 1D QCs. The quadratic invariants of a QC consist of phonon strain terms $E_{ij}E_{kl}$ which are exactly those of the crystal with the same point group, phason strain terms $W_{ij}W_{kl}$ and coupling terms $E_{ij}W_{kl}$, where $E_{ij} = (\partial_i u_j + \partial_j u_i)/2$, $W_{ij} = \partial_j w_i$, and $\boldsymbol{u}$ and $\boldsymbol{w}$ are phonon and phason displacement vectors, respectively.

A 1D QC can be described as a 3D cut of a periodic structure in four-dimensional (4D) hyperspace; hence a displacement vector in 4D space may be expressed as the direct sum of the phonon displacement $\boldsymbol{u}$ in 3D physical subspace and phason displacement $\boldsymbol{w}$ in 1D perpendicular subspace corresponding to the quasiperiodic direction of the 1D QC. This indicates that the phason displacement vector $\boldsymbol{w}$ for 1D QCs has only one component w_3 and hence there are only three phason strains W_{31}, W_{32} and W_{33} for 1D QCs compared with nine phonon strains $E_{ij}(i, j = 1, 2, 3)$. Therefore, in the elastic constant matrix $[CKR]$ (Ding *et al* 1993), the matrix $[C]$ is just the same as the stiffness elastic constant matrix of the corresponding crystal structure, $[K]$ is a 3×3 matrix and $[R]$ is a 9×3 matrix due to the possible coupling invariants between E_{ij} and $W_{3l}(R_{ij3l})$. From the viewpoint of group representation theory, both ∂_j and u_j transform under a 3D representation Γ_A, while w_3 does so under an 1D representation Γ_B. The latter may be an identity representation, or sometimes be a 1D non-identity representation with a character 1 for the first-type operations and a character -1 for the second-type operations. The number of independent elastic constants

for every point group can be calculated by the method of Yang *et al* (1994). The quadratic elastic invariants are then derived by the method described by Yang *et al* (1995b).

According to the above rules and the generalized elasticity theory (Ding *et al* 1993), we shall give all the quadratic invariants, elastic energies, Hooke's law and equilibrium equations for 1D QCs. As a general form, the elastic energy, generalized Hooke's law and equilibrium equations of 1D QC can be written as follows: the elastic energy density is

$$f = \tfrac{1}{2}[E_{11}, E_{22}, E_{33}, E_{23}, E_{31}, E_{12}, E_{32}, E_{13}, E_{21}, W_{33}, W_{31}, W_{32}]\begin{bmatrix} C & R \\ R^T & K \end{bmatrix}\begin{bmatrix} E_{11} \\ E_{22} \\ E_{33} \\ E_{23} \\ E_{31} \\ E_{12} \\ E_{32} \\ E_{13} \\ E_{21} \\ W_{33} \\ W_{31} \\ W_{32} \end{bmatrix} \tag{8}$$

the generalized Hooke's law is

$$T_{ij} = C_{ijkl}E_{kl} + R_{ij3l}W_{3l} \qquad (i, j, k, l = 1, 2, 3) \tag{9}$$

$$H_{3j} = R_{kl3j}E_{kl} + K_{3j3l}W_{3l} \tag{10}$$

and the static equilibrium equations are

$$C_{ijkl}\partial_j\partial_l u_k + R_{ij3l}\partial_j\partial_l W_3 + f_i = 0 \tag{11}$$

$$K_{3j3l}\partial_j\partial_l W_3 + R_{kl3j}\partial_j\partial_l u_k + g_3 = 0. \tag{12}$$

4.1. Triclinic system

In the triclinic 1D QC system, the point group may be 1 or $\bar{1}$, and the invariants up to quadratic order include $E_{11}, E_{22}, E_{33}, E_{23}, E_{31}, E_{12}, W_{31}, W_{32}$ and W_{33} and their mutual products. It is clear that there are $n_C = 21$ independent elastic constants in $[C]$ as in the triclinic crystal system, $n_K = 6$ in $[K]$ because of $K_{3j3l} = K_{3l3j}$, and $n_R = 18$ in $[R]$ because $R_{ij3l} = R_{ji3l}$. Therefore, the total number of independent elastic constants $n_C + n_K + n_R = 21 + 6 + 18 = 45$ (listed in the fourth column of table 2).

4.2. Monoclinic system

In the monoclinic 1D QC system, there are two Laue classes, i.e. $2/m_h(2, m_h, 2/m_h)$ and $2_h/m(2_h, m, 2_h/m)$. The unique axis of the point groups $2, m_h$ and $2/m_h$ is the z axis; hence the invariants up to quadratic order are

$$E_{11}, E_{22}, E_{33}, E_{12}, E_{23}^2, E_{31}^2, E_{23}E_{31}; W_{33}, W_{31}^2, W_{32}^2, W_{31}W_{32}; E_{23}W_{31}, E_{23}W_{32}, E_{31}W_{31}, E_{31}W_{32}. \tag{13}$$

Table 2. Systems, Laue classes, point groups, numbers of independent elastic constants and space groups for 1D QCs.

System	Laue class	Point group	Numbers of independent elastic constants $n_C + n_K + n_R$	Space group	
				Hermann–Mangnin symbol	Number in *International Tables*
Triclinic	$\bar{1}$	1	$21 + 6 + 18$	$P1$	1
		$\bar{1}$		$P\bar{1}$	2
Monoclinic	$2/m_h$	2	$13 + 4 + 8$	$P112$	3
		m_h		$P11m$	6
				$P11b$	7
		$2/m_h$		$P112/m$	10
				$P112/b$	13
	$2_h/m$	2_h	$13 + 4 + 10$	$P121$	3
				$P12_11$	4
				$C121$	5
		m		$P1m1$	6
				$P1a1$	7
				$C1m1$	8
		$2_h/m$		$P12/m1$	10
				$P12_1/m1$	11
				$C12/m1$	12
				$P12/a1$	13
				$P12_1/a1$	14
Orthorhombic	mmm_h	2_h2_h2	$9 + 3 + 5$	$P222$	16
				$P2_122$	17
				$P2_12_12$	18
				$C222$	21
		$mm2$		$Pmm2$	25
				$Pbm2$	28
				$Pba2$	32
				$Cmm2$	35
		2_hmm_h		$P2mm$	25
				$P2_1am$	26
				$P2_1ma$	26
				$P2aa$	27
				$P2mb$	28
				$P2_1ab$	29
				$P2an$	30
				$P2_1mn$	31
				$C2mm$	38
				$C2mb$	39
		mmm_h		$Pmmm$	47
				$Pmaa$	49
				$Pban$	50
				$Pbmm$	51
				$Pmma$	51
				$Pbmn$	53
				$Pbaa$	54
				$Pbam$	55
				$Pmab$	57
				$Pmmn$	59
				$Cmmm$	65
				$Cmma$	67

Table 2. (Continued)

System	Laue class	Point group	Numbers of independent elastic constants $n_C + n_K + n_R$	Space group	
				Hermann–Mangnin symbol	Number in *International Tables*
Tetragonal	$4/m_h$	4	$7+2+4$	$P4$	75
		$\bar{4}$		$P\bar{4}$	81
		$4/m_h$		$P4/m$	83
				$P4/n$	85
	$4/m_hmm$	42_h2_h	$6+2+3$	$P422$	89
				$P42_12$	90
		$4mm$		$P4mm$	99
				$P4bm$	100
		$\bar{4}2_hm$		$P\bar{4}2m$	111
				$P\bar{4}2_1m$	113
				$P\bar{4}m2$	115
				$P\bar{4}b2$	117
		$4/m_hmm$		$P4/mmm$	123
				$P4/nbm$	125
				$P4/mbm$	127
				$P4/nmm$	129
Trigonal	$\bar{3}$	3	$7+2+6$	$P3$	143
		$\bar{3}$		$P\bar{3}$	147
	$\bar{3}m$	32_h	$6+2+4$	$P312$	149
				$P321$	150
		$3m$		$P3m1$	156
				$P31m$	157
		$\bar{3}m$		$P\bar{3}1m$	162
				$P\bar{3}m1$	164
Hexagonal	$6/m_h$	6	$5+2+4$	$P6$	168
		$\bar{6}$		$P\bar{6}$	174
		$6/m_h$		$P6/m$	175
	$6/m_hmm$	62_h2_h	$5+2+3$	$P622$	177
		$6mm$		$P6mm$	183
		$\bar{6}m2_h$		$P\bar{6}m2$	187
				$P\bar{6}2m$	189
		$6/m_hmm$		$P6/mmm$	191

By comparison with equation (8), we obtain the non-zero elastic constants as follows:

$$\begin{aligned} &C_{1111}, C_{2222}, C_{3333}, C_{1122}, C_{1133}, C_{1112}, C_{2233}, C_{2212}, C_{3312}, C_{3232}, C_{3231}, C_{3131}, C_{1212} \\ &K_{3333}, K_{3131}, K_{3232}, K_{3132} \\ &R_{1133}, R_{2233}, R_{3333}, R_{1233}, R_{2331}, R_{2332}, R_{3131}, R_{3132}. \end{aligned} \tag{14}$$

Therefore, the total number of independent elastic constants is

$$n_C + n_K + n_R = 13 + 4 + 8 = 25. \tag{15}$$

If the unique axis lies in the horizontal plane, e.g. along the y axis, then invariants of the point groups 2_h, m, and $2_h/m$ are

$$E_{11}, E_{22}, E_{33}, E_{31}, E_{23}^2, E_{12}^2, E_{12}E_{23}; W_{33}, W_{31}, W_{32}^2; E_{23}W_{32}, E_{12}W_{32} \tag{16}$$

and the corresponding non-zero elastic constants are

$$\begin{aligned}&C_{1111}, C_{2222}, C_{3333}, C_{1122}, C_{1133}, C_{1131}, C_{2233}, C_{2231}, C_{3331}, C_{2323}, C_{1212}, C_{3131}, C_{2312}\\ &\qquad (n_C = 13)\\ &K_{3333}, K_{3131}, K_{3331}, K_{3232}\ (n_K = 4)\\ &R_{1133}, R_{2233}, R_{3333}, R_{3133}, R_{1131}, R_{2231}, R_{3331}, R_{3131}, R_{2332}, R_{1232}\ (n_R = 10).\end{aligned} \tag{17}$$

4.3. Orthorhombic system

The point groups 2_h2_h2, $mm2$, 2_hmm_h and mmm_h in this system belong to the same Laue class. The invariants for them are

$$E_{11}, E_{22}, E_{33}, E_{23}^2, E_{31}^2, E_{12}^2; W_{33}, W_{31}^2, W_{32}^2; E_{23}W_{32}, E_{31}W_{31} \tag{18}$$

and the non-zero elastic constants are

$$\begin{aligned}&C_{1111}, C_{2222}, C_{3333}, C_{1122}, C_{1133}, C_{2233}, C_{2323}, C_{3131}, C_{1212}\ (n_C = 9)\\ &K_{3333}, K_{3131}, K_{3232}\ (n_K = 3)\\ &R_{1133}, R_{2233}, R_{3333}, R_{2332}, R_{3131}\ (n_R = 5).\end{aligned} \tag{19}$$

4.4. Tetragonal system

Two Laue classes, i.e. $4/m_h$ ($4, \bar{4}$ and $4/m_h$) and $4/m_hmm$ ($\bar{4}2_hm, 4mm, 42_h2_h$ and $4/m_hmm$), belong to this system. For the Laue class $4/m_h$ ($4, \bar{4}$ and $4/m_h$), the invariants are

$$\begin{aligned}&E_{11}+E_{22}, E_{33}, E_{23}^2+E_{31}^2, E_{12}^2, E_{11}E_{22}, E_{12}(E_{11}-E_{22}); W_{33}, W_{31}^2+W_{32}^2;\\ &\qquad E_{23}W_{32}+E_{31}W_{31}, E_{23}W_{31}-E_{31}W_{32}\end{aligned} \tag{20}$$

and the non-zero elastic constants are

$$\begin{aligned}&C_{1111}=C_{2222}, C_{3333}, C_{2323}=C_{3131}, C_{1212}, C_{1122}, C_{1133}=C_{2233}, C_{1112}=-C_{2212}\ (n_C = 7)\\ &K_{3333}, K_{3131}=K_{3232}\ (n_K = 2)\\ &R_{1133}=R_{2233}, R_{3333}, R_{2332}=R_{3131}, R_{2331}=-R_{3132}\ (n_R = 4).\end{aligned} \tag{21}$$

For the Laue class $4/m_hmm$ ($\bar{4}2_hm, 4mm, 42_h2_h$ and $4/m_hmm$), the invariants are

$$E_{11}+E_{22}, E_{33}, E_{23}^2+E_{31}^2, E_{12}^2, E_{11}E_{22}; W_{33}, W_{31}^2+W_{32}^2; E_{23}W_{32}+E_{31}W_{31} \tag{22}$$

and the non-zero elastic constants are

$$\begin{aligned}&C_{1111}=C_{2222}, C_{3333}, C_{1133}=C_{2233}, C_{1212}, C_{1122}, C_{2323}=C_{3131}\ (n_C = 6)\\ &K_{3333}, K_{3131}=K_{3232}\ (n_K = 2)\\ &R_{1133}=R_{2233}, R_{3333}, R_{2332}=R_{3131}\ (n_R = 3).\end{aligned} \tag{23}$$

4.5. Trigonal system

Two Laue classes, i.e. $\bar{3}$(3, and $\bar{3}$) and $\bar{3}m$ ($3m, 32_h$ and $\bar{3}m$), belong to the trigonal 1D QC system. For the first two point groups 3 and $\bar{3}$, the invariants include

$$\begin{aligned}&E_{11}+E_{22}, E_{33}, E_{11}E_{22}-E_{12}^2, E_{23}^2+E_{31}^2, (E_{11}-E_{22})E_{31}-2E_{23}E_{12}, (E_{11}-E_{22})E_{23}\\ &\qquad +2E_{31}E_{12}; W_{33}, W_{31}^2+W_{32}^2; (E_{11}-E_{22})W_{31}-2E_{12}W_{32}, (E_{11}-E_{22})W_{32}\\ &\qquad +2E_{12}W_{31}, E_{23}W_{32}+E_{31}W_{31}, E_{23}W_{31}-E_{31}W_{32}\end{aligned} \tag{24}$$

and the non-zero elastic constants are

$$\begin{aligned} &C_{1111} = C_{2222}, C_{3333}, C_{2323} = C_{3131}, C_{1122}, C_{1133} = C_{2233}, 2C_{1212} = (C_{1111} - C_{1122}), C_{1123} \\ &\qquad = -C_{2223} = C_{3112}, C_{2231} = C_{2312} = -C_{1131}\ (n_C = 7); \\ &K_{3333}, K_{3131} = K_{3232}\ (n_K = 2) \\ &R_{1133} = R_{2233}, R_{3333}, R_{2332} = R_{3131}, R_{2331} = -R_{3132}, R_{1131} = -R_{2231} = -R_{1232}, R_{1132} \\ &\qquad = -R_{2232} = R_{1231}\ (n_R = 6). \end{aligned} \tag{25}$$

For the latter three point groups $32_h, 3m$ and $\bar{3}m$, with $2_h \parallel \mathrm{OX}_1$ and $m \perp \mathrm{OX}_1$, the invariants $(E_{11} - E_{22})E_{31} - 2E_{23}E_{12}$, $(E_{11} - E_{22})W_{31} - 2E_{12}W_{32}$ and $E_{23}W_{31} - E_{31}W_{32}$ in (24) disappear. Therefore, in (25), we have $C_{1131} = 0$, $R_{1131} = 0$ and $R_{2331} = 0$, and hence $n_C = 6, n_K = 2$ and $n_R = 4$.

4.6. Hexagonal system

Two Laue classes, i.e. $6/m_h(6, \bar{6}$ and $6/m_h)$ and $6/m_hmm$ $(62_h2_h, 6mm, \bar{6}m2_h$ and $6/m_hmm)$, belong to the hexagonal 1D QC system. For the first three point groups, the invariants are

$$\begin{aligned} &E_{11} + E_{22}, E_{33}, E_{11}E_{22} - E_{12}^2, E_{23}^2 + E_{31}^2; W_{33}, W_{31}^2 + W_{32}^2; E_{23}W_{32} + E_{31}W_{31}, E_{23}W_{31} \\ &\qquad -E_{31}W_{32} \end{aligned} \tag{26}$$

and the non-zero elastic constants are

$$\begin{aligned} &C_{1111} = C_{2222}, C_{3333}, C_{2323} = C_{3131}, C_{1122}, C_{1133} = C_{2233}, 2C_{1212} \\ &\qquad = (C_{1111} - C_{1122})\ (n_C = 5) \\ &K_{3333}, K_{3131} = K_{3232}\ (n_K = 2) \\ &R_{1133} = R_{2233}, R_{3333}, R_{2332} = R_{3131}, R_{2331} = -R_{3132}\ (n_R = 4). \end{aligned} \tag{27}$$

For the latter four point groups with $2_h \parallel \mathrm{OX}_1$ and $m \perp \mathrm{OX}_1$, the invariants $E_{23}W_{31} - E_{31}W_{32}$ in (26) disappear. Therefore, their elastic constants are the same as (27) except that $R_{2331} = 0$. As an example, we give the actual expressions for the elastic energy, generalized Hooke's law and equilibrium equations for these four point groups, according to equations (8)–(12).

The elastic energy density is

$$f = \tfrac{1}{2}[E_{11}, E_{22}, E_{33}, 2E_{23}, 2E_{31}, 2E_{12}, W_{33}, W_{31}, W_{32}]$$

$$\times \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 & R_1 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 & R_1 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 & R_2 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 & 0 & 0 & R_3 \\ 0 & 0 & 0 & 0 & C_{44} & 0 & 0 & R_3 & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} & 0 & 0 & 0 \\ R_1 & R_1 & R_2 & 0 & 0 & 0 & K_1 & 0 & 0 \\ 0 & 0 & 0 & 0 & R_3 & 0 & 0 & K_2 & 0 \\ 0 & 0 & 0 & R_3 & 0 & 0 & 0 & 0 & K_2 \end{bmatrix} \begin{bmatrix} E_{11} \\ E_{22} \\ E_{33} \\ 2E_{23} \\ 2E_{31} \\ 2E_{12} \\ W_{22} \\ W_{31} \\ W_{32} \end{bmatrix}. \tag{28}$$

Here and subsequently we write the elastic constant C_{ijkl} in a contracted matrix notation C_{KM} as was done in the case of crystals, and we have $K_{3333} = K1$, $K_{3131} = K_{3232} = K_2$, $R_{1133} = R_{2233} = R_1$, $R_{3333} = R_2$ and $R_{2332} = R_{3131} = R_3$.

Hooke's law is

$$\begin{aligned}
T_{11} &= C_{11}E_{11} + C_{12}E_{22} + C_{13}E_{33} + R_1W_{33} \\
T_{22} &= C_{12}E_{11} + C_{11}E_{22} + C_{13}E_{33} + R_1W_{33} \\
T_{33} &= C_{13}E_{11} + C_{13}E_{22} + C_{33}E_{33} + R_2W_{33} \\
T_{23} &= T_{32} = 2C_{44}E_{23} + R_3W_{32} \\
T_{31} &= T_{13} = 2C_{44}E_{31} + R_3W_{31} \\
T_{12} &= T_{21} = 2C_{66}E_{12} \\
H_{33} &= R_1(E_{11} + E_{22}) + R_2E_{33} + K_1W_{33} \\
H_{31} &= 2R_3E_{31} + K_2W_{31} \\
H_{32} &= 2R_3E_{23} + K_2W_{32}.
\end{aligned} \tag{29}$$

The static equilibrium equations are

$$\begin{aligned}
&\partial_1(C_{11}\partial_1u_1 + C_{12}\partial_2u_2 + C_{13}\partial_3u_3) + C_{66}\partial_2(\partial_1u_2 + \partial_2u_1) + C_{44}\partial_3(\partial_1u_3 + \partial_3u_1) \\
&\qquad +(R_1 + R_3)\partial_1\partial_3w_3 + f_1 = 0 \\
&\partial_2(C_{12}\partial_1u_1 + C_{11}\partial_2u_2 + C_{13}\partial_3u_3) + C_{44}\partial_3(\partial_2u_3 + \partial_3u_2) + C_{66}\partial_1(\partial_2u_1 + \partial_1u_2) \\
&\qquad +(R_1 + R_3)\partial_2\partial_3w_3 + f_2 = 0 \\
&\partial_3(C_{13}\partial_1u_1 + C_{13}\partial_2u_2 + C_{33}\partial_3u_3) + C_{44}\partial_1(\partial_3u_1 + \partial_1u_3) + C_{44}\partial_2(\partial_3u_2 + \partial_2u_3) \\
&\qquad +[R_2\partial_3\partial_3 + R_3(\partial_1\partial_1 + \partial_2\partial_2)]w_3 + f_3 = 0 \\
&[K_1\partial_3\partial_3 + K_2(\partial_1\partial_1 + \partial_2\partial_2)]w_3 + (R_1 + R_3)\partial_3(\partial_1u_1 + \partial_2u_2) \\
&\qquad +[R_2\partial_3\partial_3 + R_3(\partial_1\partial_1 + \partial_2\partial_2)]u_3 + g_3 = 0.
\end{aligned} \tag{30}$$

5. Discussion and conclusions

Combining the possible seven types of point symmetry operations in 1D QCs, we have derived all the possible 31 1D QC point groups, which can be divided into ten Laue classes and six 1D QC systems: triclinic, monoclinic, orthorhombic, tetragonal, trigonal and hexagonal systems. Furthermore, based on the possible translations in the periodic x–y plane, 80 1D QC space groups have been derived.

It must be pointed out that 31 1D QC point groups are isomorphic with the 31 Shubnikov plane point groups (Wang and Kuo 1990, Shubnikov and Belov 1964), including ten single-coloured plane point groups, ten grey plane point groups and 11 black–white plane point groups. These 31 Shubnikov plane point groups are in turn isomorphic with 31 diffraction groups (Buxton *et al* 1976) in convergent-beam electron diffraction. Moreover, the 80 1D QC space groups are isomorphic with 80 Shubnikov plane space groups (Wang and Kuo 1990, Shubnikov and Belov 1964), including 17 single-coloured plane groups, 17 grey plane groups and 46 black–white plane groups. Goodman (1984) discussed the experimental procedure for determining these 80 Shubnikov plane groups by using convergent-beam electron diffraction.

Janssen (1992) discussed all the possible incommensurate point groups in 3D physical space obtained from the n-dimensional ($n = 4, 5, 6$) periodic structure. In table 4 of this reference, the case for $d = 3$ (dimension of physical space) and $n = 4$ (dimension of R-reducible hyperspace) corresponds to 1D QCs. There were 27 1D QC point groups. If one

distinguishes between 2 and 2_h, m and m_h, $mm2$ and $2hmm_h$, $2/m_h$ and $2h/m$ as different point groups again 31 1D QC point groups can be obtained.

In addition, we have for the first time derived numbers of independent elastic constants, as listed in the fourth column of table 2, and all the invariants up to quadratic order, for ten Laue classes of 1D QCs. This is new and complements existing work on crystals.

However, because of the presence of the phason field, the elastic behaviours of QCs are more complicated than those of crystals. An approach to phonon and phason elastic constants was made by Jaric and Nelson (1988), who have developed a theory of the x-ray diffuse scattering from QCs, which has already been used for ordinary crystals. Although some preliminary experiments have been made in this field (de Boissieu *et al* 1995), many details still have to be investigated, and only samples of a specific class, the icosahedral QCs, have been studied. Further experimental measurements of diffuse scattering in QCs are still required to obtain full information about their elastic behaviours.

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